

PhytoFit Userguide

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Initial concept, preliminary design, coding, and algorithm development/improvements

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Final app design and modifications, feature addition, new datasets, maintenance, and algorithm improvements

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Scientific support, algorithm development/improvements, review and feature recommendations

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How to cite

In publications, please include acknowledgments to **NASA OBPG** (<https://oceancolor.gsfc.nasa.gov>) for the raw satellite data and the **BIO remote sensing group** (<https://github.com/BIO-RSG>) for the application, and use this citation in the references:

Stephanie Clay, Chantelle Layton, & Emmanuel Devred. (2021). BIO-RSG/PhytoFit: First release (v1.0.0). Zenodo. <https://doi.org/10.5281/zenodo.4770754>

BibTeX format:

```
@misc{clay21,  
  author    = {Clay, Stephanie and Layton, Chantelle and Devred, Emmanuel},  
  title     = "PhytoFit",  
  howpublished = "\url{https://github.com/BIO-RSG/PhytoFit}",  
  year      = 2021  
}
```

Prerequisites

1. Install the latest versions of R and RStudio.

2. Install the necessary packages:

```
install.packages(c("fst", "shiny", "shinyWidgets", "shinyjs", "shinybusy", "leaflet", "stars", "leafem", "leafpm",  
  , "quantreg", "minpack.lm", "sp", "ggplot2", "ggpp", "dplyr", "tidyr", "raster", "curl", "sf", "fs"))  
remotes::install_github("BIO-RSG/oceancolouR")  
# if the line above doesn't work, try devtools::install_github("BIO-RSG/oceancolouR")  
# if that doesn't work, try either install.packages("remotes") or install.packages("devtools") and then run the o  
ceancolouR installation line again
```

3. Restart R after the packages have been installed.

Getting started

1. Download the PhytoFit repository (<https://github.com/BIO-RSG/PhytoFit>) one of two ways:

- a. Option 1: Code --> Download ZIP
- b. Option 2: Using git (this will make it easier to download updates in the future, by simply using the ``git pull`` command):
Open git bash terminal, navigate to the folder where you want to download the repository, and type:

```
git clone https://github.com/BIO-RSG/PhytoFit.git
```

2. Open the PhytoFit repository in Rstudio (File --> Open Project --> Navigate to the PhytoFit folder and open *PhytoFit.Rproj*)

3. Download (or update) the datasets of your choice:

Open *00_download_new_datasets.R* from the PhytoFit folder.

Set *ask_user=FALSE* to download all available datasets, or *ask_user=TRUE* to ask before downloading each one.

Alternatively, you can run the script from the command line like:

```
Rscript [script directory]/00_download_new_datasets.R 'false'
```

* set "script directory" to the full path where the script is located

* 'false' is the *ask_user* argument, set to 'true' for prompts

If you already have datasets in storage, you can update them using *00_update_datasets.R*. Set the *ask_user* argument in the script and run from RStudio, or run from the command line (e.g. `Rscript [script directory]/00_update_datasets.R 'false'`).

4. Run the app by opening *app.R* in RStudio and clicking "Run app"

WARNINGS:

- Data files will be downloaded to *data/[region]/* subfolders of the PhytoFit repository - Do **NOT** move them from there or the app will not be able to read them.
- If possible, please keep the data files if you intend to use them in the future, rather than re-downloading them later, to avoid excessive traffic on the ftp server.
- Any data that is < 3 months old is "Near Real Time" (NRT) quality. NRT data is replaced with "Science quality" data after it becomes available, following the 3-month lag. More info here: <https://lance.modaps.eosdis.nasa.gov/data/difference.php>

Troubleshooting

If you run into errors or the app crashes, try the following:

- Check if there are any helpful error messages in the console
- Clear memory: `rm(list=ls())`
- Restart R and/or RStudio
- Update packages used in the app

Main settings

1. If you have a settings file saved from a previous session, you can reapply it using this feature. **Warning: DO NOT EDIT THE SETTINGS FILE**, otherwise PhytoFit might not be able to read it properly.
2. Select your region and spatial resolution
 - Atlantic (42 to 71 °W, 39 to 63 °N)
 - Pacific (122 to 140 °W, 46 to 60 °N)
 - Gulf of Saint Lawrence (49 to 75 °W, 41 to 53 °N)
 - Baffin Bay (42 to 95 °W, 60 to 82 °N)
3. Select satellite and variable
 - Satellite sensors: MODIS-Aqua, SeaWiFS, VIIRS-SNPP, OLCI-A or B
 - Variables: Chl-a (OCI, POLY4, GSM_GS, or EOF for the Gulf region only), SST (Sea Surface Temperature)
 - **R20XX.X** indicates the reprocessing (data version). More info here: <https://oceancolor.gsfc.nasa.gov/data/reprocessing>
4. Select Chl-a concentration type and cell size model (this is applied to Chl-a before logging, if selected)
5. Select year
6. Select temporal binning (daily data is averaged over composite period before logging, if selected)
7. Select logged or unlogged data
8. Load data for the current selection of settings

Satellite Data Visualization

Option 1:

Load a file with predefined settings (.txt, created in PhytoFit): Browse to select, then click "Apply settings" and "Load data" below.

1. No file selected

Option 2:

Start selecting your settings below, then click "Load data" and adjust remaining settings as needed.

2. Region
Atlantic

3. Satellite and variable
MODIS-Aqua R2022.0, POLY4 chl-a (regional, band ratio)

View full satellite [chl-a], or use one of two models to separate satellite [chl-a] into concentrations of different phytoplankton cell sizes, and choose the cell size to view:

4. ☒ Full chlorophyll-a concentration
☐ Small/Large cell concentrations
☐ Small/Medium/Large cell concentrations

5. Year
2022

6. Data composite length
Daily

7. Log-transform data

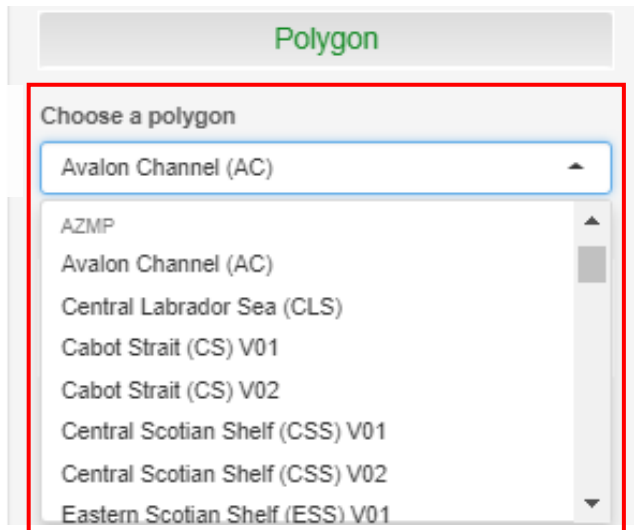
8.

Polygon selection

You can choose a polygon in order to calculate statistics and bloom metrics within that region. Click the “Polygon” button to expand this menu.

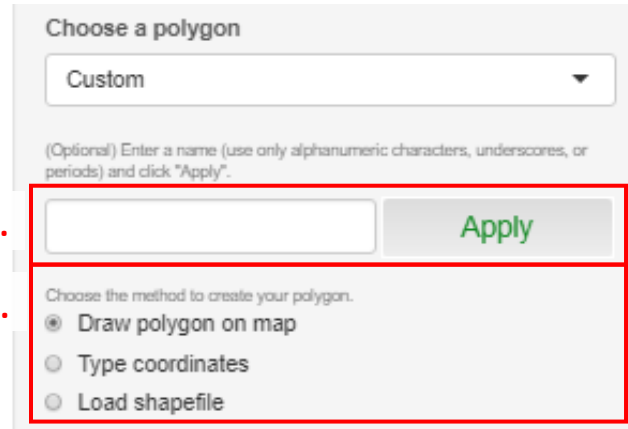
1. Choose a predefined polygon, or create your own.
2. For a custom polygon, optionally give it a name.
3. Select how you will define your custom polygon:
 - a) Draw using the controls at the top left corner of the map,
 - b) Type the coordinates, or
 - c) Select a shapefile containing a Simple Features object and click to select the polygon you want to use from the file.

1.



The screenshot shows a web interface with a tab labeled 'Polygon' in green. Below the tab is a section titled 'Choose a polygon' containing a dropdown menu. The dropdown is open, showing a list of predefined polygons: Avalon Channel (AC), AZMP, Central Labrador Sea (CLS), Cabot Strait (CS) V01, Cabot Strait (CS) V02, Central Scotian Shelf (CSS) V01, Central Scotian Shelf (CSS) V02, and Eastern Scotian Shelf (ESS) V01. The 'Avalon Channel (AC)' option is currently selected.

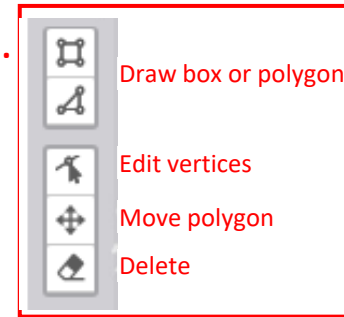
2.



The screenshot shows a dialog box titled 'Choose a polygon'. It has a dropdown menu set to 'Custom'. Below the dropdown is a text input field and an 'Apply' button. A note says: '(Optional) Enter a name (use only alphanumeric characters, underscores, or periods) and click "Apply"'. At the bottom, there is a section titled 'Choose the method to create your polygon.' with three radio button options: 'Draw polygon on map' (selected), 'Type coordinates', and 'Load shapefile'.

3.

3a.



The screenshot shows a vertical toolbar with five icons and their corresponding labels: 'Draw box or polygon' (a square with a diagonal line), 'Edit vertices' (a square with a vertex being moved), 'Move polygon' (a square with a four-way arrow), and 'Delete' (a square with an eraser). The 'Draw box or polygon' label is in red.

To close a polygon when you're done editing, click on the first point.

Only one polygon can be drawn on the map at a given time.

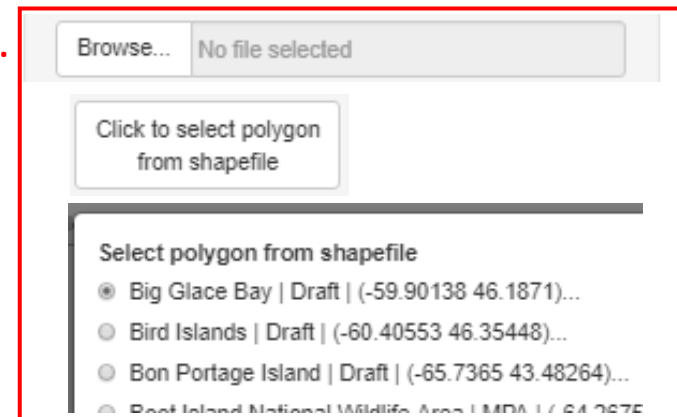
3b.



The screenshot shows a form with two text input fields. The first field is labeled 'List of latitudes:' and contains the text '42.6, 43, 42, 40.4, 40, 42.6'. The second field is labeled 'List of longitudes:' and contains the text '-61, -59, -55, -57, -60.4, -61'. Below the fields is a 'Create polygon' button.

- Decimal degrees
- Separate coordinates by commas
- Use latitude/longitude < 0 for west/south

3c.



The screenshot shows a web interface for selecting a polygon from a shapefile. It has a 'Browse...' button and a 'No file selected' status. Below is a button that says 'Click to select polygon from shapefile'. Underneath is a section titled 'Select polygon from shapefile' with a list of options, each preceded by a radio button. The options are: 'Big Glace Bay | Draft | (-59.90138 46.1871)...', 'Bird Islands | Draft | (-60.40553 46.35448)...', 'Bon Portage Island | Draft | (-65.7365 43.48264)...', and 'East Island National Wildlife Area | MPA | (-64.2675 46.1871)...'. The first option is selected.

- Select the “shp” file and all files with the same name but different extensions (e.g. dbf, sbn, sbx, shx, prj, qix...)
- If the polygon has a large number of vertices, it might take several seconds to load.

Statistics

Click the “Statistics” button to expand this menu.

1. Select the minimum percent coverage required for a point in the time series to be used in the bloom fitting procedure or displayed in the density plot. If a daily (or 4-day, 8-day) composite has insufficient coverage within your polygon, it will be ignored.
2. Select the outlier detection method.
 - mean \pm 2 standard deviations
 - mean \pm 3 standard deviations
 - median \pm 1.5 * interquartile range
 - Outer percentiles (0.01%, 0.1%, ...)
3. Select the statistic (mean or median) to use to summarize data within your polygon for each day (or 4-day or 8-day period).
4. To exclude data outside a certain range, enter the values here and click “apply”. Data outside this range will not be included in the statistics or bloom fit. To ignore a boundary, leave it blank.

The screenshot shows a web interface for the 'Statistics' menu. It contains four sections, each with a red box and a number indicating a step:

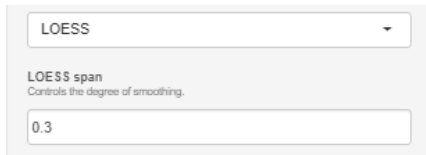
- 1.** A text input field containing the value '10'. Above it is the heading 'Minimum % coverage.' and a note: 'Composites with lower coverage in the selected polygon will not be plotted on the density plot or time series, or used in the model fit.'
- 2.** A dropdown menu showing 'None'. Above it is the heading 'Outlier detection method' and subtext: 'SD = standard deviation' and 'IQR = interquartile range'.
- 3.** A dropdown menu showing 'Arithmetic mean'. Above it is the heading 'Statistic' and a note: 'Calculate either the mean or median value of each composite, to be used in the time series and model fit.'
- 4.** Two empty text input fields separated by a minus sign, followed by a green 'Apply' button. Above it is the heading 'Range of pixel values' and a note: 'Choose the range of values allowed in the calculation of the statistics and model fit (pixels outside this range will be omitted). If a limit is left blank, it will be ignored.'

Model (bloom) fit

Click the “Model fit” button to expand this menu.

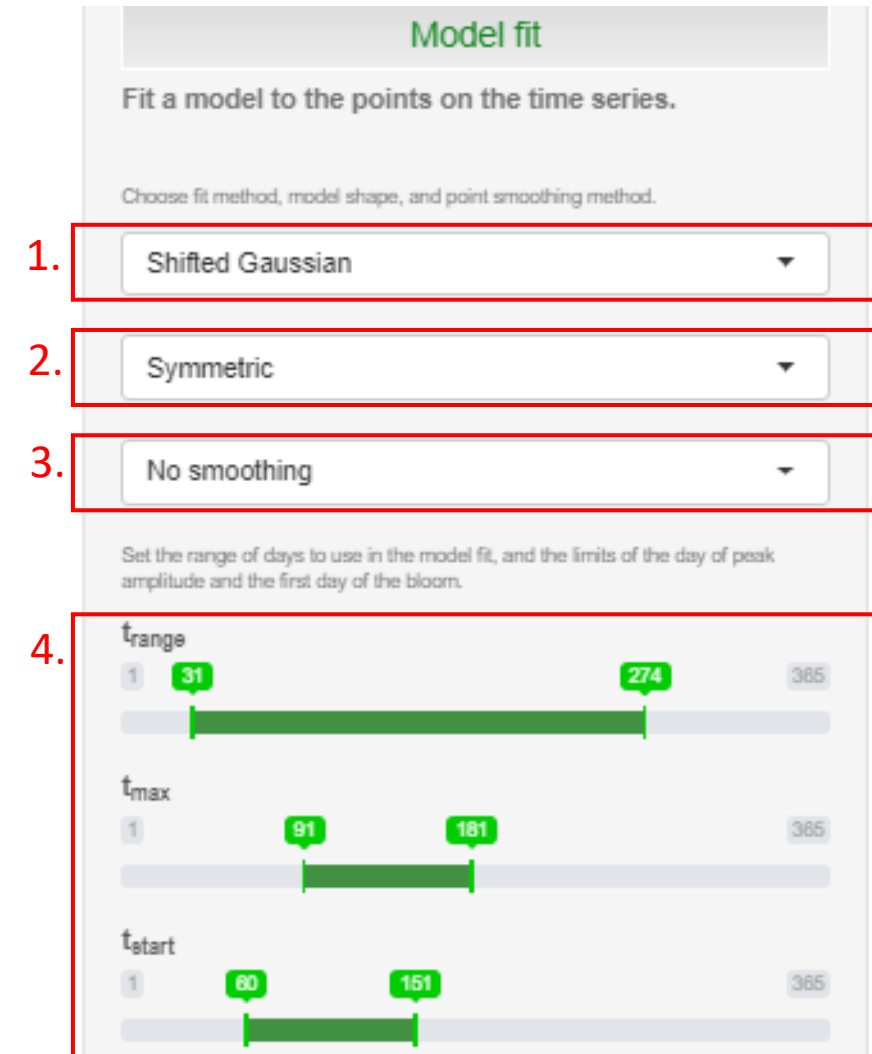
Each point in the time series and bloom fit is the daily (or 4-day, 8-day) spatial average (or median) of data after removal of outliers and points outside the desired range, using the binned data values. Only points with sufficient percent coverage inside the polygon on that day/week are used, within the range of days selected by the user.

1. Select the model to use in your fit. *Default = Shifted Gaussian*
2. Select the model shape around the bloom peak timing.
3. Choose whether to smooth points using LOESS (locally estimated scatterplot smoothing) in the time series before fitting or just fit the raw data points. If you smooth the points, you must also set the “span”, which controls the degree of smoothing:



A screenshot of the LOESS span control interface. It features a dropdown menu with 'LOESS' selected. Below it, a text input field is labeled 'LOESS span' with the subtitle 'Controls the degree of smoothing.' and contains the value '0.3'.

4. Adjust the range of days to use in the fit, and restrict to a certain time window to search for the peak timing or start of the bloom period. t_{start} and t_{max} will be restricted based on t_{range} .



A screenshot of the 'Model fit' interface. The title 'Model fit' is in green. Below it, the text 'Fit a model to the points on the time series.' is followed by 'Choose fit method, model shape, and point smoothing method.' There are three dropdown menus, each with a red number and a red box around it: 1. 'Shifted Gaussian', 2. 'Symmetric', and 3. 'No smoothing'. Below these, the text 'Set the range of days to use in the model fit, and the limits of the day of peak amplitude and the first day of the bloom.' is followed by three sliders, each with a red number and a red box around it: 4. t_{range} (range 1 to 365, green bar from 31 to 274), t_{max} (range 1 to 365, green bar from 91 to 181), and t_{start} (range 1 to 365, green bar from 60 to 151).

Model (bloom) fit (continued)

5. If you are modelling with a Shifted Gaussian, there are more options:

- a) t_{start} calculation method
 - % amplitude: Define t_{start} as the day when the curve reaches a specified percentage of its amplitude over the background value, or
 - Constant threshold: Define t_{start} as the day when the curve reaches a specified threshold over the background value.
- b) t_{max} switch
If this is ON, the bloom peak timing is allowed to vary as a parameter within the nonlinear least squares fitting procedure, rather than being a fixed value based on the actual maximum value.
WARNING: t_{start} can't be restricted if this is set to ON, because the t_{start} limits are set by restricting σ (the parameter controlling the width of the curve) relative to a known t_{max} value.
- c) βt switch
If this is ON, the background line of the curve is allowed to vary linearly with time.
- d) weights
If this is ON, points in the fit are weighted by the percent coverage inside the polygon.
- e) Remove background
If this is checked, the background data line will be subtracted from the data points / curve before calculating the amplitude and magnitude.
- f) Fits are flagged (unaffected but marked) if the following occurs:
 - Flag 1: Flagged if $\text{amplitude}_{\text{fit}} / \text{amplitude}_{\text{real}}$ is outside the selected range
 - Flag 2: Flagged if $\text{magnitude}_{\text{fit}} / \text{magnitude}_{\text{real}}$ is outside the selected range
 - Flag 3: Flagged if $\sigma \leq \text{temporal composite length}$ (i.e. 1, 4, or 8 days)
 - Flag 4: Flagged if the calculated t_{start} is on the boundary of the t_{start} slider
 - Flag 5: Flagged if the calculated t_{max} is on the boundary of the t_{max} slider
 - Flag 6: Flagged if the calculated t_{end} is on the boundary of the t_{range} sliderYou can adjust the range of acceptable ratio limits for flags 1 and 2 and click "apply".

6. If you are modelling with the Threshold method, set the threshold coefficient.

t_{start} is defined as the point where chlorophyll-a drops below the threshold for > 14 days, measuring the days/weeks backward from the day of maximum concentration.

$\text{threshold} = (\text{threshold coefficient}) * (\text{median data value})$

$\text{median data value} = \text{median of all points used in bloom fit (within day range, with sufficient \% coverage)}$

5a. ☒ % amplitude
☐ Constant threshold
Set % curve amplitude to mark start of bloom.
20 %
Switch to ON to consider t_{max} as a parameter in the regression.
WARNING: This will disable t_{start} limits.

5b. t_{max} OFF
Switch to ON to allow background values to vary linearly as a function of day.

5c. βt OFF
Switch to ON to weight each point in the time series by percent coverage.

5d. weights OFF
When calculating magnitude (area under the curve between t_{start} and t_{end}) and amplitude of the curve, should the background be removed first?

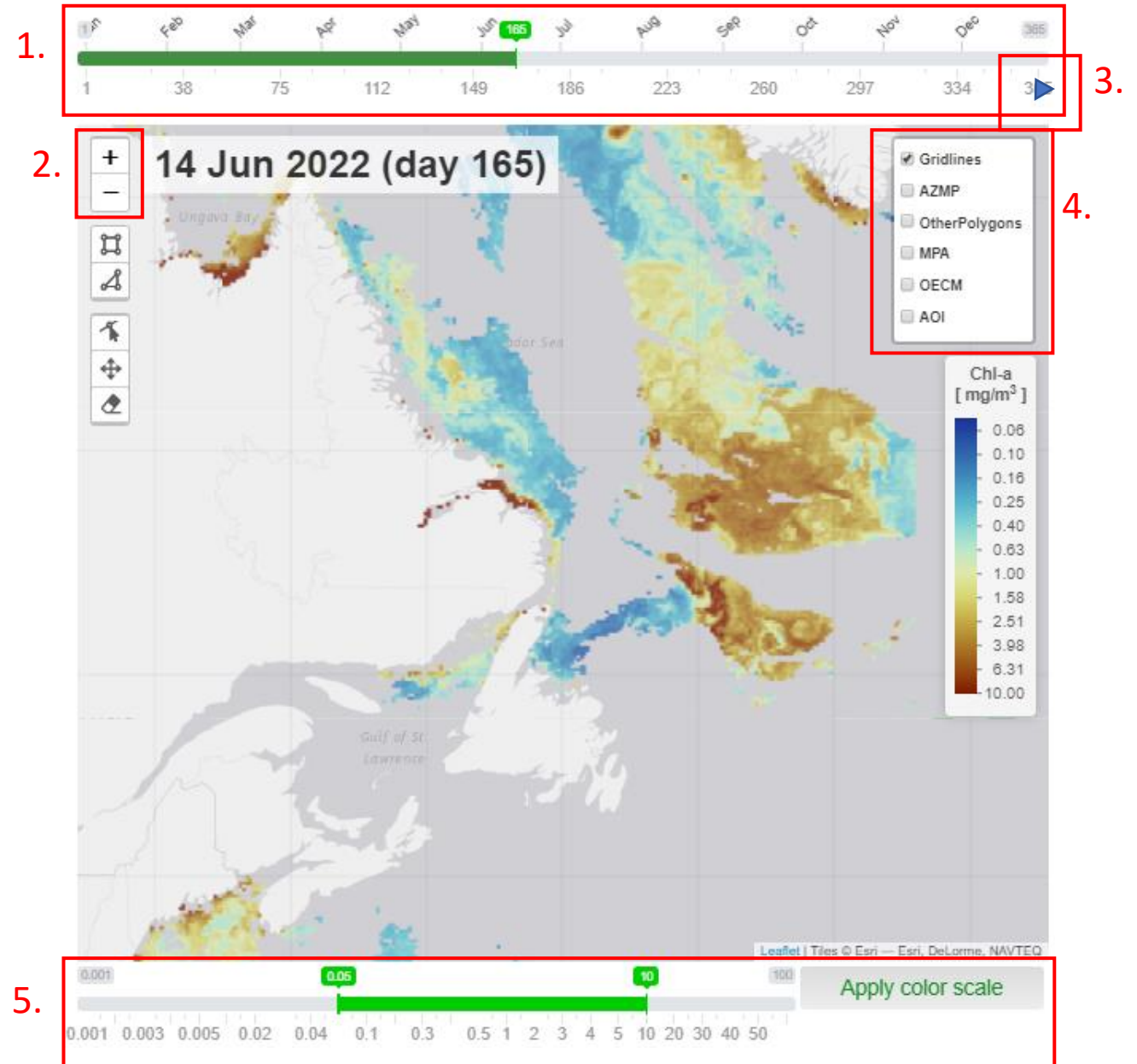
5e. ☒ Remove background
Flags
Fits will be flagged if they meet certain criteria that indicate potential problems with the fit (NOTE: this does not affect the fit itself). Combinations of flags will be written as a single number (for example, 13 for flags 1 and 3). Click below for details.
Optionally adjust the parameters of some flags.

5f. Flag descriptions
Flag 1: Amplitude ratio limits
0.75 - 1.25 Apply
Flag 2: Magnitude ratio limits
0.85 - 1.15 Apply

6. Threshold coefficient
The start of the phytoplankton bloom is considered to be the point before t_{max} when [chl a] drops below a threshold for > 14 days.
Threshold = $\text{chl a}_{\text{median}} * \text{threshold coefficient}$
1.05

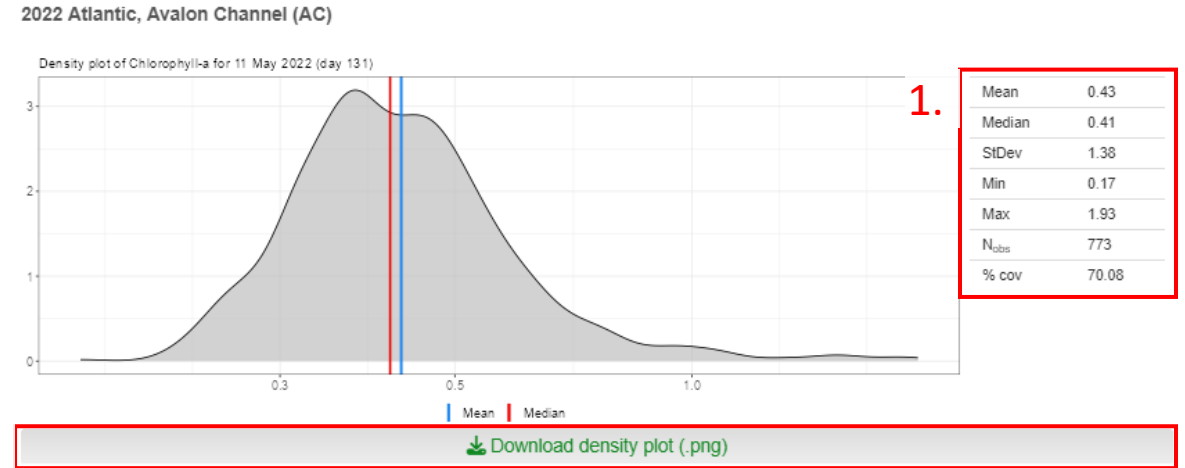
Output and display - Map

1. Day selector – Move the slider to view the satellite imagery for that day (or 4-day or 8-day period)
2. Map zoom functions
3. Play button to allow map to load images in sequence with a 4-second delay between each image
4. Toggle groups of predefined polygons on the map, for viewing only
5. Adjust the color scale on the map



Output and display – Density plot

1. Daily (or 4-day, 8-day) statistics within your polygon
2. Click here to download this density plot with the table of statistics overlaid on the plot



Output and display – Time series plot

1. Instruction to double-click the center of a point in the time series to load the satellite imagery and density plot for that point
2. Annual statistics, model parameters, and model metrics within your polygon
3. Download this time series plot with the table of stats and metrics overlaid
4. Download a csv file containing the table of statistics within your polygon for each day (or 4-day, 8-day period) for the selected year
5. Download a table with the model parameters and metrics



Model fits – Shifted Gaussian

$$B = B_0 + \beta t + \left(\frac{h}{\sqrt{2\pi}\sigma} \right) \exp\left(-\frac{(t - t_{\max})^2}{2\sigma^2} \right)$$

B_0 , β , h , and σ are calculated using nonlinear least squares.
 t_{\max} is also calculated this way if the t_{\max} switch is ON.

This is done with the *minpack.LM::nlsLM* function in R, which uses the Levenberg-Marquardt method. Starting guesses are required for the variables listed above (4 different sets of starting guesses are attempted during the fit), and lower/upper limits are enforced. If the curve is asymmetric, the same limits and guesses are used for each side. If the data is logged, B_0 limits and starting guesses are also logged.

If a Gaussian curve can't be fitted to the points, a failure code will be given in the output. These are the code meanings:

- Code 1: not enough data in the selected limits
- Code 2: nls failed
- Code 3: t_{start} threshold too high
- Code 4: t_{start} too early (before day 1)
- Code 5: t_{start} outside t_{range}
- Code 6: t_{end} outside t_{range}
- Code 7: data at end of bloom period is > threshold

Parameter	Units	Description	Lower limit	Upper limit	Starting guesses			
					1	2	3	4
B	mg.m ⁻³	Vector of data points in the time series						
t	Day of year	Vector of days, same length as B						
B ₀	mg.m ⁻³	Background data value	0	5	0.5			
β (beta)	mg.m ⁻³ .day ⁻¹	Linear rate of change of B ₀	-0.02	0.01	-0.002	-0.002	0.001	0.001
h	Unitless	Controls the height of the curve	0	350	50	50	10	10
σ (sigma)	Unitless	Controls the width of the curve	0	100	10	2	2	1
t _{max}	Day of year	Day of maximum B	User-selected	User-selected	Day of maximum data value (within t _{max} limits)			

Model fits – Shifted Gaussian (continued)

$$B = B_0 + \beta t + \left(\frac{h}{\sqrt{2\pi}\sigma} \right) \exp\left(-\frac{(t - t_{max})^2}{2\sigma^2} \right)$$

Several metrics are collected, relating to the timing of the bloom and total data values. Some metrics are calculated using both the Gaussian curve and the real data points.

Metric	Units	Description
t_{start}	Day	Start of the bloom
t_{max_real}	Day	Timing of maximum value within bloom period
t_{max_fit}	Day	Timing of peak of Gaussian curve
t_{end}	Day	End of the bloom
$t_{duration}$	Day	Duration of the bloom
$Amplitude_{real}$	$mg.m^{-3}$	Maximum value within bloom period
$Magnitude_{real}$	$mg.m^{-3}.day$	Area under the real data points within the bloom period
$Amplitude_{fit}$	$mg.m^{-3}$	Peak of Gaussian curve
$Magnitude_{fit}$	$mg.m^{-3}.day$	Area under the Gaussian curve within the bloom period

- If "remove background" has been checked, the background data will be subtracted before calculating amplitude and magnitude.
- If points between t_{start} and t_{end} are below the background line and "remove background" has been selected, the magnitude (area) below the line will be negative so it will be subtracted from the final value (this only affects $Magnitude_{real}$).
- If LOESS smoothing and point-weighting are both selected, the LOESS-smoothed curve will be calculated using the weighted real data points. The curve is then fit to the LOESS values. Note that in this case, the mean, median, $Amplitude_{real}$, and $Magnitude_{real}$ are still calculated using the real data values.

Model fits – Rate of Change

This algorithm does not model a curve like the Shifted Gaussian, but only calculates the maximum, start, and end days of the bloom.

The maximum is selected as the day of actual maximum concentration, within the selected range.

The initiation is the day of the maximum rate of change in concentration, within the selected bounds.

If any indices cannot be computed, they will be blank and not appear on the time series plot. This might happen due to an insufficient number of data points in the time series, or within the range of days allowed for the start or day of maximum concentration of the bloom.

B_0 (the background data value) is computed using the R function *quantreg::rq* to perform a quantile regression (25th percentile) on the full dataset (days/weeks with sufficient percent coverage), and is subtracted from the data to calculate the final amplitude and magnitude metrics.

Metric	Units	Description
t_{start}	Day	Start of the bloom
$t_{\text{max_real}}$	Day	Timing of maximum value within bloom period
t_{end}	Day	End of the bloom
t_{duration}	Day	Duration of the bloom
$\text{Amplitude}_{\text{real}}$	mg.m^{-3}	Maximum value within bloom period
$\text{Magnitude}_{\text{real}}$	$\text{mg.m}^{-3}.\text{day}$	Area under the real data points within the bloom period

- If LOESS smoothing and point-weighting are both selected, the LOESS-smoothed curve will be calculated using the weighted real data points.

Model fits – Threshold

This model is similar to the Rate of Change:

- It only calculates the maximum, start, and end days of the bloom
- B_0 is calculated using *quantreg::rq* and subtracted from the data points to get amplitude and magnitude
- The maximum is selected as the day of actual maximum concentration, within the selected range.

The initiation is defined as the day the data drops below a threshold for > 14 consecutive days, working backward from the day of the maximum value.

If your data are not logged:

Threshold = (Threshold coefficient) * (median data used in the fit)

If your data are logged:

Threshold = log10 [(Threshold coefficient) * 10^{(median log10(data) used in the fit)}]

Threshold coefficient = user-selected

Metric	Units	Description
t_{start}	Day	Start of the bloom
$t_{\text{max_real}}$	Day	Timing of maximum value within bloom period
t_{end}	Day	End of the bloom
t_{duration}	Day	Duration of the bloom
Amplitude _{real}	mg.m ⁻³	Maximum value within bloom period
Magnitude _{real}	mg.m ⁻³ .day	Area under the real data points within the bloom period

- If LOESS smoothing and point-weighting are both selected, the LOESS-smoothed curve will be calculated using the weighted real data points.

Run full time series and save settings

At the bottom of the left panel, you have the option of collecting statistics and fitting the model for multiple years of data, and downloading the collection of results in a zip file.

1. Check these boxes if you want to include the time series plots in png format in the output, and the table of statistics in csv format.
2. Adjust the slider to the range of years you want to process.
3. Select the polygons you want to use in the processing.
4. Click “Run time series” to run the calculations, then
5. Click “Download results” to download the zip file, which uses the following naming convention:
satellite_region_compositeLength_years_cellSizes_variable_fitmethod_timecreated
6. Save a settings file for the current selection of settings.

The screenshot shows the 'Time series' section of a web application. It includes a list of checkboxes for output formats, a year range slider, a polygon selection dropdown, and three action buttons. Red boxes and numbers 1-6 highlight specific elements as described in the instructions.

Time series
Select a series of years and the polygons you would like to process using the current settings, then click "Run time series" to generate the following:

1. ☒ time series plots (.png),
☒ tables of statistics (.csv),
☒ a single .csv file containing the fitted parameters for all selected years and polygons, and
☒ a .csv file containing the settings used for the time series, for reference.

Files will be zipped to a folder following the naming convention `satellite_region_compositeLength_years_cellSizes_variable_fitmethod_timecreated`.
Make sure at least one polygon is selected.
When processing is complete and the new filename appears over the download button, click "Download results (.zip)".

2. A slider for selecting years, with green markers at 2002 and 2023.
3. A dropdown menu labeled "Select your polygons" with "Custom" selected.
4. A button labeled "Run time series".
5. A button labeled "Download results (.zip)".
6. A button labeled "Save settings (.txt)".

AZMP fitting parameters

Annual reporting for the AZMP (Atlantic Zone Monitoring Program, <https://www.dfo-mpo.gc.ca/science/data-donnees/azmp-pmza/index-eng.html>) includes statistics and bloom metrics for a set of polygons. Previously, AZMP boxes were typically fitted using a Fortran script, examining and adjusting every fit manually. Results were stored here: <ftp://ftp.dfo-mpo.gc.ca/bometrics/spring-bloom>. Below are the settings to use in PhytoFit to most closely replicate these fitting procedures. Unavoidable differences between the original procedure and PhytoFit are highlighted in red.

L2 and L3 flag info here: <https://oceancolor.gsfc.nasa.gov/resources/atbd/ocl2flags>

	Original Fortran bloom fitting system	PhytoFit bloom fitting
Sensor	VIIRS-SNPP	VIIRS-SNPP
Spatial resolution	~1km	4km
Projection	Equidistant cylindrical	Binned
Level-2 flags	All L2 flags except TURBIDW	L3 flags + FILTER
Chl-a model	OCI, not logged	OCI, not logged
Temporal binning	Weekly (using a 4-week-per-month system)	8-day
Minimum % coverage	1%	1%
Outliers	Not removed	Not removed
Statistic	Average	Average
Range of pixel values	$\leq 64 \text{ mg.m}^{-3}$	$\leq 64 \text{ mg.m}^{-3}$
Model	Symmetric Shifted Gaussian No smoothing, no point weighting, flat background (i.e. beta OFF), t_{max} defined as day of max concentration (i.e. t_{max} switch OFF)	Symmetric Shifted Gaussian No smoothing, no point weighting, flat background (i.e. beta OFF), t_{max} defined as day of max concentration (i.e. t_{max} switch OFF)
Range of days used in fit	Feb-July, or Feb-Aug for boxes $\geq 56^\circ\text{N}$	t_{range} 31-212 (boxes $< 56^\circ\text{N}$), 31-244 (boxes $\geq 56^\circ\text{N}$)
Gaussian fit flags	Box has $< 10\%$ coverage, flags 1-3 listed in PhytoFit	[See 6 flags listed in Shifted Gaussian description]
t_{start} calculation	20% curve amplitude	20% curve amplitude
Bloom metrics	Remove background before calculating amplitude, magnitude	Remove background before calculating amplitude, magnitude

Extra tools

In the tools subfolder of the repository, there are a few extra R scripts:

Scripts to create your own region and predefined polygons:

- `tools_01a_define_polygons.R`
- `tools_01b_create_new_region.R`

Scripts to concatenate and format the output from PhytoFit:

- `tools_02_format_bloommetrics.R`

- `tools_fit_bloom_from_chla.R`

This standalone script can accept a dataframe with year, doy, and chl columns, and fit a bloom to the chl using the same settings as used in the app.

This is useful for fitting blooms to in situ data records that only have one value per day or week.

To use this script on your own computer, you must also download ``functions.R``, ``gaussFit.R``, ``threshold.R``, and ``rateOfChange.R``.

Required packages: ``dplyr``, ``oceancolouR`*`, ``minpack.lm``

Optional packages for plotting results: ``ggplot2``, ``patchwork``

*The `oceancolouR` package, which can be installed with one of the following commands in R:

```
remotes::install_github("BIO-RSG/oceancolouR", build_vignettes = TRUE)
devtools::install_github("BIO-RSG/oceancolouR", build_vignettes = TRUE)
```

References and data sources

- Bloom fitting models (Shifted Gaussian, Rate of Change, and Threshold methods) :
Layton, C., Devred, E., DeTracey B.. 2022. A comparison of phytoplankton spring bloom fitting methods using MODIS satellite-derived chlorophyll-a concentration for the Maritimes region. Can. Tech. Rep. Hydrogr. Ocean Sci. 340: vii + 22 p.
https://publications.gc.ca/collections/collection_2022/mpo-dfo/Fs97-18-340-eng.pdf
- Chlorophyll-a algorithm **OCx**:
O'Reilly, John & Maritorena, S. & Mitchell, B.G. & Siegel, David & Carder, Kendall & Garver, S.A. & Kahru, Mati & McClain, Charles. (1998). Ocean color chlorophyll algorithms for SeaWiFS. Journal of Geophysical Research. 103. 937-953.
https://www.researchgate.net/publication/284463756_Ocean_color_chlorophyll_algorithms_for_SeaWiFS
- Chlorophyll-a algorithm **GSM**:
Maritorena, Stéphane & Siegel, David & Peterson, Alan. (2002). Optimization of a semianalytical ocean color model for global-scale application. Applied optics. 41. 2705-14. 10.1364/AO.41.002705.
https://www.researchgate.net/publication/11345370_Optimization_of_a_semianalytical_ocean_color_model_for_global-scale_application
- Chlorophyll-a algorithms **OCI**, **POLY4**, and **GSM_GS** (regional tuning):
Clay, S.; Peña, A.; DeTracey, B.; Devred, E. Evaluation of Satellite-Based Algorithms to Retrieve Chlorophyll-a Concentration in the Canadian Atlantic and Pacific Oceans. Remote Sens. 2019, 11, 2609.
<https://www.mdpi.com/2072-4292/11/22/2609>
- Chlorophyll-a algorithm **EOF**:
Laliberté, J.; Larouche, P.; Devred, E.; Craig, S. Chlorophyll-a Concentration Retrieval in the Optically Complex Waters of the St. Lawrence Estuary and Gulf Using Principal Component Analysis. Remote Sens. 2018, 10, 265.
<https://www.mdpi.com/2072-4292/10/2/265>

References and data sources (continued)

- Phytoplankton cell size model 1 (small/large cells):
Devred, Emmanuel & Sathyendranath, S & Stuart, V & Maass, H & Ulloa, Osvaldo & Platt, T. (2006). A two-component model of phytoplankton absorption in the open ocean: Theory and applications. *Journal of Geophysical Research*. 111. 10.1029/2005JC002880.
https://www.researchgate.net/publication/229086123_A_two-component_model_of_phytoplankton_absorption_in_the_open_ocean_Theory_and_applications
- Phytoplankton cell size model 2 (small/medium/large cells):
Devred, Emmanuel & Sathyendranath, Shubha & Stuart, Venetia & Platt, Trevor. (2011). A three component classification of phytoplankton absorption spectra: Application to ocean-color data. *Remote Sensing of Environment - REMOTE SENS ENVIRON*. 115. 2255-2266. 10.1016/j.rse.2011.04.025.
https://www.researchgate.net/publication/251494326_A_three_component_classification_of_phytoplankton_absorption_spectra_Application_to_ocean-color_data
- Phytoplankton cell size models (updated coefficients):
Liu, Xiaohan & Devred, Emmanuel & Johnson, Catherine. (2018). Remote Sensing of Phytoplankton Size Class in Northwest Atlantic from 1998 to 2016: Bio-Optical Algorithms Comparison and Application. *Remote Sensing*. 10. 10.3390/rs10071028.
https://www.researchgate.net/publication/326033452_Remote_Sensing_of_Phytoplankton_Size_Class_in_Northwest_Atlantic_from_1998_to_2016_Bio-Optical_Algorithms_Comparison_and_Application#pf18
- Raw data:
Daily level-3 binned files are downloaded from NASA OBPG (<https://oceancolor.gsfc.nasa.gov>), and weekly composites are generated by taking a simple arithmetic average of each pixel over the selected composite period (e.g. 4 days or 8 days). The binned data is used for statistics and bloom fitting, projected onto a regular grid on the map for display.
 - NASA OCI chlorophyll-a algorithm: https://oceancolor.gsfc.nasa.gov/resources/atbd/chlor_a
 - Level-3 binned files: <https://oceancolor.gsfc.nasa.gov/l3>
 - Binning scheme: <https://oceancolor.gsfc.nasa.gov/resources/docs/format/l3bins>
 - Level-2 and 3 default flags: <https://oceancolor.gsfc.nasa.gov/resources/atbd/ocl2flags>
(PhytoFit data uses these default flags + FILTER flag)